EXHIBIT 1

Insight II

An Integrated Modeling Environment

MBO(N)D is a multibody dynamics program which allows you to produce simulations of molecular movements and properties up to 20 times faster than conventional methods.

MODELER automatically generates a refined homology model of a protein, given only the sequence alignment to a known 3D protein structure. You are able to generate excellent structural models given as little as 30% homology to known structures.

NMR Refine DGII provides an entry-level option into NMR refinement software with capabilities for generating structures from NMR-derived distance and dihedral restraints. The DG II, Restraint Analysis, NMR Database and ProStat pulldowns combine to give the NMR spectroscopist the necessary tools for generating, analyzing and verifying high resolution structures.

NMR Refine Advanced expands the refinement capabilities found in NMR Refine DG II to include simulated annealing and restrained molecular mechanics and dynamics (MD Schedule), refinement of NOE intensities using hybrid-matrix approaches (IRMA), direct refinement of NOE volumes (NOE-MD), an interface to back-calculating 2D NOESY crosspeak intensities (NOE Simulate), and a spreadsheet method of analyzing NMR-related structural and dynamical molecular parameters (Query).

NMR X-PLOR streamlines the steps in structure determination from NMR data. You can visualize your NMR restraints, directly set up and launch X-PLOR refinement calculations and evaluate the quality of the calculated structures.

Profiles-3D searches a structural-motif database with a new sequence, looking for compatibility; searches a sequence database with an example structure, seeking similarity; or verifies the agreement between the sequence and current model of a protein sequence/structure under study.

QuantaMM combines quantum mechanical and force field methods, allowing you to use accurate first-principles methods to study cluster models while taking the surrounding environment fully into account. Enables highly accurate simulations of active sites and systems such as metallo-proteins.

Search/Compare generates and compares the conformers of different molecules. You can operate on molecular fields and volumes, superimpose two or more molecules, and search systematically for sterically allowed conformations.

Sketcher is used to draw molecules in 2D and automatically convert them to 3D models.

Turbomole applies Hartree-Fock and density functional methods to predict molecular structure and energetics and numerous properties such as electrostatic potentials, molecular moments, and polarizabilities.

X-PLOR/DG is a macromolecular structure determination program that integrates NMR experimental data with molecular mechanics, dynamics and energy minimization to aid in the solution of three dimensional structures. This includes distance geometry, simulated annealing, restrained molecular dynamics, and relaxation matrix analysis.

X-PLOR/Refine is an X-ray structure determination program that integrates crystallographic diffraction data with molecular mechanics, dynamics and energy minimization to aid in the solution of three-dimensional structures.

Xsight integrates all of the major computational techniques for macromolecular crystallography. You can analyze and interpret X-ray data, build models of protein structures and relate them to electron density, refine structures against X-ray data, analyze structures for symmetry, and visualize and validate structures.

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- Perform searches to find structures of interest.
- See your spreadsheet data dynamically update as you change the geometry of the molecular structure.

Docking

Docking allows independent manipulation of molecules with interactive non-bond energy calculations.

- Manipulate molecules and collections of molecules, to perform docking exploration with bump checking.
- Calculate the interaction between two molecules using explicit van der Waals energy and/or Coulombic energy.
- Use an energy grid to quickly calculate the interaction energy between two molecules.

Hardware Requirements

Insight II versions available for Silicon Graphics and IBM RISC System/6000 workstations.

Software Tools

Modules in the Insight II environment provide solutions for X-ray and NMR structure determination, protein modeling, dynamics simulation and analysis, docking and structure-based drug design.

Affinity provides automated docking of ligands to receptors in the structure-based drug design process. These calculations include an implicit solvation term. The component effects of this solvation term and of other energetic partitions can be viewed graphically.

Biopolymer constructs models of peptides, proteins, carbohydrates, and nucleic acids for visualizing complex macromolecular structures.

CFF, an advanced Class II Force field, is used to optimize DNA, RNA, carbohydrates, lipids, proteins, peptides, and small-molecule models, giving a high confidence level for calculations in drug discovery, protein design, genomic therapeutics, NMR spectroscopy, and X-ray crystallography.

CHARMm combines standard minimization and dynamics capabilities with expert features including free energy perturbation (FEP), correlation analysis and combined quantum and molecular mechanics (QM/MM) methods.

Consensus builds a 3D model of a protein from its amino acid sequence and the known structures of related proteins using distance constraints derived from the reference protein structures.

Converter converts 2D structural databases into 3D structural databases.

DelPhi is a powerful and flexible program for high-level analysis of molecular structure and the results of molecular dynamics simulations.

DelPhi calculates electrostatic potentials and solvation energies of both large and small molecules, including nucleic acids. You can use DelPhi to rigorously examine the effects of charge distribution, ionic strength, and dielectric constant on the electrostatic potentials of macromolecules.

Discover incorporates a range of well validated forcefields for dynamics simulations, minimization, and conformational searches, allowing you to predict the structure, energetics and properties of organic, inorganic, organometallic, and biological systems.

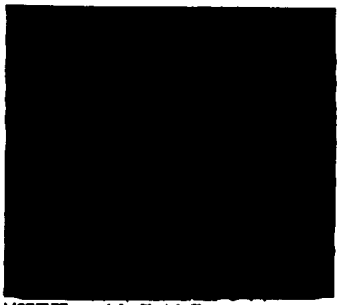
DMol is a quantum mechanics module which makes possible, fast, reliable, quantitative predictions of molecular structure, energetics and properties for ground and transition states. DMol employs advanced density functional theory (DFT).

Homology builds a 3D model of a protein from its amino acid sequence and the known structure of related proteins. Standard techniques of backbone building, loop modeling, structural overlay and statistical analysis of the resulting models are available.

Ludi is a powerful tool for de novo rational drug design. Ludi can be used to fit molecules into the active site of a receptor by identifying and matching complementary polar and hydrophobic groups.

Ludi/ACD links the design tools of Ludi to MDL's Available Chemicals Directory. Ludi/ACD provides access to over 65,000 commercially available structures to accelerate your search for drug candidates.

MADSYS is a program that provides phasing of multi-wavelength anomalous dispersion (MAD) data collected at synchrotron radiation X-ray sources.



MODELER, a module of Insight II, can create homology models in an automated fashion. The resulting models can be visualized and analyzed via Insight II's graphical interface.

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